THE PRECISE EQUILIBRIUM STRUCTURE DETERMINATION OF CHLOROBENZENE (C_6H_5Cl) BY ROTATIONAL SPECTROSCOPY

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The rotational spectra of over 30 isotopologues of chlorobenzene (C_6H_5Cl, C_{2v}) have been collected over portions of the 2 – 360 GHz frequency region. The transitions of these isotopologues were least-squares fit to complete sextic Hamiltonians with the support of computationally predicted spectroscopic constants. The resultant rotational constants of all available isotopologues, alongside high-level computational corrections for vibration-rotation interaction and electron-mass distribution, were used to determine a highly precise semi-experimental equilibrium (r_e^{SE}) structure of chlorobenzene. Finally, advanced quantum mechanical calculations were performed at the CCSD(T)/cc-pCV5Z level to compare to the experimental results. Analysis of the chlorobenzene r_e^{SE} structure will provide insight into the limitations of molecular structure determination when some atoms lie close to (or directly on) principal axes, a difficulty observed in previous molecular structure determinations.